Convergence Analysis of Meshfree Approximation Schemes

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Abstract

This work is concerned with the formulation of a general framework for the analysis of meshfree approximation schemes and with the convergence analysis of the Local Maximum-Entropy (LME) scheme as a particular example. We provide conditions for the convergence in Sobolev spaces of schemes that are *n-consistent*, in the sense of exactly reproducing polynomials of degree less or equal to $n \geq 1$, and whose basis functions are of *rapid decay*. The convergence of the LME in $W^{1,p}_{\text{loc}}(\Omega)$ follows as a direct application of the general theory. The analysis shows that the convergence order is linear in h, a measure of the *density* of the point set. The analysis also shows how to parameterize the LME scheme for optimal convergence. Because of the convex approximation property of LME, its behavior near the boundary is singular and requires additional analysis. For the particular case of polyhedral domains we show that, away from a small singular part of the boundary, any Sobolev function can be approximated by means of the LME scheme. With the aid of a capacity argument, we further obtain approximation results with truncated LME basis functions in $H^1(\Omega)$ and for spatial dimension $d > 2$.

1 Introduction

Meshfree approximation schemes (cf., e. g., [13] for a review) are advantageous in a number of areas of application, e. g., those involving Lagrangian descriptions of unconstrained flows (cf., e. g., [16] for a representative example) where methods based on triangulation, such as the finite-element method, inevitably suffer from problems of mesh-entanglement. The present work is concerned with the formulation of a general framework for the analysis of meshfree approximation schemes (cf., e. g., [17] for representative past work) and with its application to the Local Maximum-Entropy (LME) scheme as an example. By way of conceptual backdrop, we may specifically envision time-independent problems for which the solutions of interest follow as the minimizers of a functional $F\colon X \to \bar{\mathbb{R}}$, where X is a topological vector space. General conditions for the existence of solutions are provided by the Tonelli's theorem (e. g., [10]). In this framework, an approximation scheme is a sequence X_k of subspaces of X, typically of finite dimension, defining a corresponding sequence of *Galerkin reductions* of F,

$$F_k(u) = \begin{cases} F(u), & \text{if } u \in X_k, \\ +\infty, & \text{otherwise.} \end{cases} \tag{1}$$

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An approximation scheme is then said to be *convergent* if it has the following density property: For every $u \in X$, there exists a sequence $u_k \in X_k$ such that $\lim_{k\to\infty} u_k = u$. The connection between density of the approximation scheme and convergence is provided by the following proposition [7].

Proposition 1. *Let X be endowed with two metrizable topologies S and T, with T finer than S. Let $F\colon X \to \bar{\mathbb{R}}$ be coercive in (X, S) and continuous in (X, T). Let X_k be a dense sequence of sets in (X, T) and let F_k be the corresponding sequence of Galerkin reductions of F. Then the sequence F_k Γ-converges to the lower semicontinuous envelope of F and is equicoercive in (X, S).*

We recall that Γ-convergence is a powerful notion of variational convergence of functionals that, in particular, implies convergence of minimizers. Thus, if the sequence F_k is equicoercive, then the minimizers of F are accumulation points of minimizers of F_k, i. e., if $F_k(u_k) = \inf F_k$ then the sequence u_k has a subsequence that converges to a minimizer of F. We also recall that the topology T is finer than S, i. e., any converging sequence for T converges for S. In applications, T is typically a metric or normed topology and S the corresponding weak topology.

It thus follows that, within the general framework envisioned here, the analysis of convergence of approximation schemes reduces to ascertaining the density property. Towards this end, in Section 3 we begin by analyzing meshfree approximation schemes that are *n-consistent*, in the sense of exactly reproducing polynomials of degree less or equal to $n \geq 1$, and whose basis functions are of *rapid decay*. Specifically, for schemes subordinate to point sets possessing a certain geometrical regularity property that we term *h-density*, we prove a uniform error bound for consistent and rapidly-decaying approximation schemes. In addition, we show that the sets of functions spanned by consistent and rapidly-decaying approximation schemes are dense in Sobolev spaces.

In Sections 4 and 5, we apply the general results of Section 3 to the Local Maximum-Entropy (LME) approximation scheme of Arroyo and Ortiz [2] (see also [3, 27, 9, 12]). The LME scheme has been extensively assessed numerically over a broad range of test problems [2, 18, 16], but a rigorous convergence analysis has been heretofore unavailable. The general theory of Section 3 readily establishes the density of the LME approximation spaces X_k in $W^{1,p}_{\mathrm{loc}}(\Omega)$, cf. Section 4. In particular, the analysis shows that the convergence order is linear in h, a measure of the *density* of the point set. These convergence rates and the corresponding error bounds are in agreement with the numerical results reported in [2], and are comparable to those of the first-order finite element method (cf., e. g., [5]). Conveniently, the analysis also shows how to choose the LME *temperature parameter* so as to obtain optimal convergence. This optimal choice is in agreement with that determined in [2, 16] by means of numerical testing.

The LME scheme is a *convex approximation scheme* in which the basis functions are constrained to take non-negative values. By virtue of this restriction, the LME scheme is defined for convex domains only. Consequently, its behavior near the boundary is somewhat singular and requires careful additional analysis. In Section 5, for the particular case of polyhedral domains we show that, away from a small singular part of the boundary, any Sobolev function can indeed be approximated by means of the LME scheme. Then, with the aid of a capacity argument we obtain approximation results with truncated LME basis functions in $H^1(\Omega)$ and for spatial dimension $d > 2$.

2 Prolegomena

The open d-ball $B(x, \delta)$ of radius δ centered at x is the set $\{y \in \mathbb{R}^d \colon |y - x| < \delta\}$. The closed d-ball $\bar{B}(x, \delta)$ of radius δ centered at x is the set $\{y \in \mathbb{R}^d \colon |y - x| \leq \delta\}$. Given a set $A \subset \mathbb{R}^d$, we

denote by $\bar{A}$ its closure, and by ∂A its boundary. By a *domain* we shall specifically understand an open and bounded subset of $\mathbb{R}^d$. Given a *point set* $P \in (\mathbb{R}^d)^N$, we denote by $\overline{\mathrm{conv}}(P)$ its closed convex hull [20], and by $\mathrm{conv}(P)$ the interior of $\overline{\mathrm{conv}}(P)$. We recall that a *$d$-simplex* $T \subset \mathbb{R}^d$ is the convex hull of $d+1$ affinely independent points [20]. Given a bounded set $A \subset \mathbb{R}^d$, its *size* h_A is the diameter of the smallest ball containing A.

The following definitions formalize the notion of a point set $P \subset \Omega$ that approximates a domain Ω uniformly.

Definition 1 (h-covering)**.** *We say that a point set $P \subset \mathbb{R}^d$ is an* h-covering *of a set $A \subset \mathbb{R}^d$, $h > 0$, if for every $x \in A$ there exists a d-simplex T_x of size $h_{T_x} < h$ and with vertices in P such that $x \in T_x$.*

Definition 2 (h-density)**.** *We say that a point set $P \subset \mathbb{R}^d$ has* h-density *bounded by $\tau > 0$ if for every $x \in \mathbb{R}^d$, $\#\big(P \cap \bar{B}(x,h)\big) \leq \tau$.*

For a point set $P \subset \Omega$ with h-density bounded by τ, the following proposition bounds its number of points in rings of $\mathbb{R}^d$.

Proposition 2. *Assume $P \subset \Omega$ has h-density bounded by τ, for some h, $\tau > 0$. Then there is a constant $c > 0$ that depends on τ and d such that,*

$$\#\left(P \cap \left(\bar{B}(x,th) \setminus B(x,(t-1)h)\right)\right) \leq c\,t^{d-1}, \tag{2}$$

$\forall x \in \Omega$ and integers $t \geq 1$.

Proof. Let

$$\begin{aligned} E_1 &= \left\{ y \in \mathbb{R}^d \colon \mathrm{dist}\left(y, \bar{B}(x,th) \setminus B(x,(t-1)h)\right) \leq h \right\} \\ &= \bar{B}(x,(t+1)h) \setminus B(x,(t-2)h) \end{aligned} \tag{3}$$

and

$$\begin{aligned} E_2 &= \left\{ y \in \mathbb{R}^d \colon \mathrm{dist}\left(y, \bar{B}(x,th) \setminus B(x,(t-1)h)\right) \leq 2h \right\} \\ &= \bar{B}(x,(t+2)h) \setminus B(x,(t-3)h). \end{aligned} \tag{4}$$

Then for every $y \in \bar{B}(x,th) \setminus B(x,(t-1)h)$ there is a $z \in Z := E_1 \cap hd^{-\frac{1}{2}}\mathbb{Z}^d$ such that $|y - z| \leq h$ and so

$$\bar{B}(x,th) \setminus B(x,(t-1)h) \subset \bigcup_{z \in Z} \bar{B}(z,h). \tag{5}$$

On the other hand, $z + [0, hd^{-\frac{1}{2}})^d \subset E_2$ for all $z \in Z$, and thus

$$\#Z h^d d^{-\frac{d}{2}} = \left| \bigcup_{z \in Z} z + [0, hd^{-\frac{1}{2}})^d \right| \leq |E_2| \leq |B(0,1)| h^d \left((t+2)^d - (t-3)^d \right) \leq c h^d t^{d-1}. \tag{6}$$

Consequently,

$$\#\left(P \cap \left(\bar{B}(x,th) \setminus B(x,(t-1)h)\right)\right) \leq \#\left(P \cap \bigcup_{z \in Z} \bar{B}(z,h) \right) \leq c d^{\frac{d}{2}} \tau t^{d-1}. \tag{7}$$

$\square$

3 Convergence Analysis of General Meshfree Approximation Schemes

In this Section we analyze meshfree approximation schemes that are n-consistent and whose shape functions are of *rapid decay*. Specifically, we prove a uniform error bound for consistent and rapidly-decaying approximation schemes. In addition, we show that the set of functions spanned by consistent and rapidly-decaying approximation schemes are dense in Sobolev spaces.

Let $\Omega \subset \mathbb{R}^d$ be a domain. By an approximation scheme $\{I, W, P\}$ we mean a collection $W = \{w_a,\ a \in I\}$ of shape functions and a point set P, both indexed by I. Given an approximation scheme $\{I, W, P\}$, we approximate functions $u \colon \Omega \to \mathbb{R}$ by functions in the span X of W of the form

$$u_I(x) = \sum_{a \in I} u(x_a) w_a(x), \tag{8}$$

provided that this operation is well defined. More generally, we shall consider sequences of approximation schemes $\{I_k, W_k, P_k\}$ and let

$$u_k(x) = \sum_{a \in I_k} u(x_a) w_a(x), \tag{9}$$

be the corresponding sequence of approximations to u in the sequence X_k of finite-dimensional spaces of functions spanned by W_k. We note that, for simplicity, we assume that all functions are defined over a common domain Ω. Depending on the approximation scheme, this assumption may implicitly restrict the type of domains that may be considered, e. g., polyhedral domains. The aim then is to ascertain conditions on the approximation scheme under which $u_k \to u$ in an appropriate Sobolev space $W^{m,p}(\Omega)$.

We recall the following definition of consistency of approximation schemes [23].

Definition 3 (Consistency)**.** *We say that an approximation scheme $\{I, W, P\}$ is consistent of order $n \geq 0$, or n-consistent, relative to a point set P if it exactly interpolates polynomials of degree less or equal to n within Ω, i. e., if*

$$x^\alpha = \sum_{a \in I} x_a^\alpha w_a(x) \tag{10}$$

for all multiindices α of degree $|\alpha| \leq n$.

A simple binomial expansion shows that (10) can equivalently be replaced by

$$\sum_{a \in I} w_a(x) = 1, \tag{11a}$$

$$\sum_{a \in I} w_a(x)(x_a - x)^\alpha = 0,\ \forall \alpha \in \mathbb{N}^d,\ 0 < |\alpha| \leq n, \tag{11b}$$

in the definition of consistency.

Consistency results in a number of identities involving the partial derivatives of the shape functions, which we record next for subsequent use (cf. [6]).

Lemma 1. *Let $\{I, W, P\}$ be an approximation scheme. Suppose that W consists of $C^r(\Omega)$ shape-functions that are nth-order consistent relative to P in Ω. Let α, β be multiindices, with $0 \leq |\alpha| \leq n$, $0 \leq |\beta| \leq r$. Then,*

$$\sum_{a \in I} D^\beta w_a(x)(x_a - x)^\alpha = \begin{cases} \alpha!, & \text{if } \alpha = \beta, \\ 0, & \text{otherwise.} \end{cases} \tag{12}$$

Proof. We proceed by induction on $|\beta|$. For $\beta = 0$, the identity (12) follows directly from consistency. Let $0 \leq m < r$ and assume eq. (12) holds for all multiindices α, β such that $0 \leq |\beta| \leq m$ and $0 \leq |\alpha| \leq n$. Let β and γ be such that $|\beta| = m$ and $|\gamma| = 1$. Then, for $\alpha = 0$ we have, by consistency,

$$\sum_{a \in I} D^{\beta+\gamma} w_a(x) = D^{\beta+\gamma} \sum_{a \in I} w_a(x) = 0, \tag{13}$$

whereas for $0 < |\alpha| \leq n$ we have, also by consistency,

$$\begin{aligned} &\sum_{a \in I} D^{\beta+\gamma} w_a(x)(x_a - x)^\alpha \\ &= D^\gamma \sum_{a \in I} D^\beta w_a(x)(x_a - x)^\alpha + \sum_{a \in I} D^\beta w_a(x)(\alpha \cdot \gamma)(x_a - x)^{\alpha-\gamma} \\ &= (\alpha \cdot \gamma) \sum_{a \in I} D^\beta w_a(x)(x_a - x)^{\alpha-\gamma} \end{aligned} \tag{14}$$

Suppose that $\alpha \neq \beta + \gamma$. Then, from (12),

$$\sum_{a \in I} D^\beta w_a(x)(x_a - x)^{\alpha-\gamma} = 0. \tag{15}$$

Suppose, contrariwise, that $\alpha = \beta + \gamma$. Then, also from (12),

$$(\alpha \cdot \gamma) \sum_{a \in I} D^\beta w_a(x)(x_a - x)^{\alpha-\gamma} = (\alpha \cdot \gamma)(\alpha - \gamma)! = \alpha!, \tag{16}$$

whereupon (14) becomes

$$\sum_{a \in I} D^{\beta+\gamma} w_a(x)(x_a - x)^\alpha = \alpha!, \tag{17}$$

and (12) holds for all multiindices β of degree $m + 1$. $\square$

We recall that the Taylor approximation of order r of a function $u \in C^{r+1}(\Omega)$ at $y \in \Omega$ is

$$T_r(u)(x, y) = \sum_{|\alpha| \leq r} \frac{1}{\alpha!} D^\alpha u(x)(y - x)^\alpha \tag{18}$$

and its remainder is

$$R_{r+1}(x, y) = u(y) - T_r(u)(x, y), \tag{19}$$

which turns out to be

$$R_{r+1}(x, y) = \sum_{|\alpha| = r+1} \frac{1}{\alpha!} D^\alpha u\big(x + \theta(y - x)\big)(y - x)^\alpha, \tag{20}$$

for some $\theta \in (0, 1)$.

Functions in the span of a consistent shape-function basis satisfy the following *multipoint Taylor formula* (cf. [5, 6]).

Proposition 3 (Multipoint Taylor formula)**.** *Let W be a $C^r(\Omega)$ shape-function set nth-order consistent relative to a point set P in Ω, $u \in C^{\ell+1}(\mathrm{conv}(\Omega))$ and $m = \min\{n, \ell\}$. Then,*

$$D^\alpha u_I(x) = D^\alpha u(x) + \sum_{a \in I} R_{m+1}(x_a, x) D^\alpha w_a(x). \tag{21}$$

for all $|\alpha| \leq \min\{m, r\}$ and $x \in \Omega$.

Proof. The proof follows that of Theorem 1 of [6]. From the Taylor expansion of order m of u at x we have

$$u(x_a) = \sum_{|\beta| \leq m} \frac{1}{\beta!} D^\beta u(x)(x_a - x)^\beta + R_{m+1}(x, x_a). \tag{22}$$

whence it follows that

$$\begin{aligned} D^\alpha u_I(x) &= \sum_{a \in I} u(x_a) D^\alpha w_a(x) \\ &= \sum_{a \in I} \left(\sum_{|\beta| \leq m} \frac{1}{\beta!} D^\beta u(x)(x_a - x)^\beta + R_{m+1}(x, x_a) \right) D^\alpha w_a(x) \\ &= \sum_{|\beta| \leq m} \frac{1}{\beta!} D^\beta u(x) \left(\sum_{a \in I} D^\alpha w_a(x)(x_a - x)^\beta \right) + \sum_{a \in I} R_{m+1}(x, x_a) D^\alpha w_a(x), \end{aligned} \tag{23}$$

and (21) follows from Lemma 1. $\square$

We recall that a function $f \in C^\infty(\mathbb{R}^d)$ is said to be *rapidly decreasing* if [21]

$$\sup_{|\alpha| \leq N} \sup_{x \in \mathbb{R}^d} (1 + |x|^2)^N |(D^\alpha f)(x)| < \infty \tag{24}$$

for all $N = 0, 1, 2, \ldots$, where $|x|^2 = \sum x_i^2$.

The next definition formalizes a polynomial-decay condition of the shape functions and their derivatives.

Definition 4 (Approximation scheme with polynomial decay)**.** *We say that an approximation scheme $\{I, W, P\}$ has a* polynomial decay of order (r, s) *for constants $c > 0$ and $h > 0$ if the basis W is in $C^r(\Omega)$, and*

$$\sup_{|\alpha| \leq r} \sup_{x \in \Omega} \sup_{a \in I} \left(1 + \left| \frac{x - x_a}{h} \right|^2 \right)^s h^{|\alpha|} |D^\alpha w_a(x)| < c. \tag{25}$$

A sequence of approximation schemes $\{I_k, W_k, P_k\}$ has a uniform polynomial decay of order (r, s) *if there exists a constant $c > 0$ and a sequence $h_k \to 0$ such that, for each k, $\{I_k, W_k, P_k\}$ has a polynomial decay of order (r, s) for constants c and h_k.*

We note that, if the shape functions are invariant under a linear transformation, then the left hand side of (25) is also invariant under the same transformation change.

The next proposition establishes a key concentration property of approximation schemes with polynomial decay.

Proposition 4 (Shape-function concentration)**.** *Let $\{I, W, P\}$ be an approximation scheme. Suppose that there exists $\tau > 0$ such that P has h-density bounded by τ. Suppose, in addition, that the approximation scheme has polynomial decay of order (r, s) for constants $c > 0$ and h, with $2s > d$. Then, for every $\theta > 0$ there exists a constant $c_\theta > 0$ such that*

$$\sum_{x_a \in P \setminus \bar{B}(x, c_\theta h)} |w_a(x)| \leq \theta, \tag{26}$$

everywhere in Ω.

Proof. For every nonnegative integer $t \geq 1$, let $U_t(x)$ be the ring of node points $U_t(x) = \{x_a \in P \colon (t-1)h \leq |x_a - x| < th\}$. Note that $P = \cup_{t=1}^{\infty} U_t(x)$. By Proposition 2, there exists a constant c' that depends on τ and d such that, for any $t \geq 1$, the number of node points of $U_t(x)$ is at most $\# U_t(x) \leq c' t^{d-1}$. Since the approximation scheme has polynomial decay of order (r, s) with $2s > d$, for any integer $c_\theta \geq 1$ we have

$$\begin{aligned}\sum_{x_a \in P \setminus \bar{B}(x, c_\theta h)} |w_a(x)| &\leq \sum_{t=c_\theta}^{\infty} \sum_{x_a \in U_t(x)} |w_a(x)| \leq \sum_{t=c_\theta}^{\infty} c' t^{d-1} c((t-1)^2 + 1)^{-s} \leq \sum_{t=c_\theta}^{\infty} c' t^{d-1} c t^{-2s} \\ &\leq \sum_{t=c_\theta}^{\infty} c' c t^{-1-(2s-d)}.\end{aligned} \tag{27}$$

Note that the series $\sum_{t=1}^{\infty} c' c t^{-1-(2s-d)}$ is finite. In particular, there exists a value $c_\theta < \infty$, depending on d, τ, and θ, such that $\sum_{t=c_\theta}^{\infty} c' c t^{-1-(2s-d)} \leq \theta$. □

For an n-consistent approximation scheme with sufficiently high polynomial decay, the following theorem provides a uniform interpolation error bound.

Theorem 1 (Uniform interpolation error bound)**.** *Let $\{I, W, P\}$ be an approximation scheme. Suppose that:*

i) The approximation scheme is n-consistent, $n \geq 0$.

ii) There exists $\tau > 0$ such that P has h-density bounded by τ.

iii) The approximation scheme has polynomial decay of order (r, s) with $2s > d + m + 1$, where $m = \min\{n, \ell\}$.

Let $u \in C^{\ell+1}(\overline{\mathrm{conv}}(\Omega))$. Then, there exists a constant $C < \infty$ such that

$$|D^\alpha u_I(x) - D^\alpha u(x)| \leq C \left\| D^{m+1} u \right\|_\infty h^{m+1-|\alpha|}, \tag{28}$$

for every $|\alpha| \leq \min\{m, r\}$ and $x \in \Omega$.

Proof. By Proposition 3,

$$|D^\alpha u_I(x) - D^\alpha u(x)| \leq \sum_{a \in I} |R_{m+1}(x_a, x)| \, |D^\alpha w_a(x)| \tag{29}$$

for every multiindex α of degree less or equal to $\min\{m, r\}$ and every $x \in \Omega$. Next, we proceed to bound the right-hand side of this inequality. For each nonnegative integer $t \geq 1$, let $U_t(x)$ be

the ring of nodal points $U_t(x) = \{x_a \in P\colon (t-1)h \leq |x_a - x| < th\}$. Note that $P = \cup_{t=1}^{\infty} U_t(x)$. By Proposition 2, there exists a constant c that depends on τ and d such that, for any $t \geq 1$, the number of node points of $U_t(x)$ is at most $\# U_t(x) \leq c t^{d-1}$. In addition, from (20) we have

$$|R_{m+1}(x_a, x)| \leq \frac{d^{m+1}}{(m+1)!} \left\| D^{m+1} u \right\|_{\infty} (th)^{m+1}. \tag{30}$$

By the assumption of polynomial decay there exists a constant $0 < c' < \infty$ such that

$$|D^{\alpha} w_a(x)| \leq c' \left(\left| \frac{x - x_a}{h} \right|^2 + 1 \right)^{-s} h^{-|\alpha|} \leq c' \left((t-1)^2 + 1 \right)^{-s} h^{-|\alpha|} \leq 5 c' t^{-2s} h^{-|\alpha|}, \tag{31}$$

for every $x_a \in U_t(x)$. From the preceding bounds we have

$$\begin{aligned}
&\sum_{a \in I} |R_{m+1}(x_a, x)| \, |D^{\alpha} w_a(x)| \\
&= \sum_{t=1}^{\infty} \sum_{x_a \in U_t(x)} |R_{m+1}(x_a, x)| \, |D^{\alpha} w_a(x)| \\
&\leq \sum_{t=1}^{\infty} \sum_{x_a \in U_t(x)} \frac{d^{m+1}}{(m+1)!} \left\| D^{m+1} u \right\|_{\infty} (th)^{m+1} 5 c' t^{-2s} h^{-|\alpha|} \\
&\leq 5c' \frac{d^{m+1}}{(m+1)!} \left\| D^{m+1} u \right\|_{\infty} h^{m+1-|\alpha|} \sum_{t=1}^{\infty} \# U_t(x) \, t^{m+1-2s} \\
&\leq 5c' \frac{d^{m+1}}{(m+1)!} \left\| D^{m+1} u \right\|_{\infty} h^{m+1-|\alpha|} \sum_{t=1}^{\infty} c t^{d-1} t^{m+1-2s} \\
&\leq 5c' c \frac{d^{m+1}}{(m+1)!} \left\| D^{m+1} u \right\|_{\infty} h^{m+1-|\alpha|} \sum_{t=1}^{\infty} t^{d+m-2s}.
\end{aligned} \tag{32}$$

Since $d + m - 2s < -1$, it follows that $\sum_{t=1}^{\infty} t^{d+m+1-2s} < \infty$. Thus,

$$|D^{\alpha} u_I(x) - D^{\alpha} u(x)| \leq C \left\| D^{m+1} u \right\|_{\infty} h^{m+1-|\alpha|}, \tag{33}$$

for every $x \in \Omega$, where we note that the constant $C = 5c' c \frac{d^{m+1}}{(m+1)!} \left(\sum_{t=1}^{\infty} t^{d+m-2s} \right)$ depends on τ, d, c', and s. $\square$

The following corollaries to Theorem 1 show that a function in $W^{m,p}(\Omega)$ can be approximated by means of consistent approximation schemes of polynomial decay.

Corollary 1. *Under the assumptions of Theorem 1,*

$$\|u_I - u\|_{W^{j,p}(\Omega)} \leq C \|D^{m+1} u\|_{\infty} h^{1+m-j}, \tag{34}$$

for $1 \leq p < \infty$, $j = \min\{n, r, \ell\}$ *and every* $u \in C^{\ell+1}(\overline{\mathrm{conv}}(\Omega))$.

Proof. By Theorem 1, there exists a constant $0 < C < \infty$ such that,

$$\|u_I - u\|_{C^j(\bar{\Omega})} \leq C \|D^{m+1} u\|_\infty h^{1+m-j}, \tag{35}$$

so that the assertion follows from the continuous embedding $C^j(\bar{\Omega}) \hookrightarrow W^{j,p}(\Omega)$. $\square$

Convergence in $W^{j,p}(\Omega)$ finally follows from standard theory of approximation by continuous functions (cf. e. g., [1]). For completeness, we proceed to note a particular case of practical relevance. We recall that a domain Ω satisfies the *segment condition* if, for all x in the boundary of Ω, there exists a neighborhood U_x and a direction $y_x \neq 0$ such that, for any point $z \in \bar{\Omega} \cap U_x$, the point $z + t y_x$ belongs to Ω, for all $0 < t < 1$ ([1], §3.21). Convex domains satisfy the segment condition without additional restrictions on their boundaries. We additionally recall ([1], thm. 3.22) that, if Ω satisfies the segment condition, then the functions of $C_c^\infty(\mathbb{R}^d)$ restricted to Ω are dense in $W^{j,p}(\Omega)$ for $1 \leq p < \infty$.

Corollary 2. *Let Ω be a domain satisfying the segment condition. Suppose that the assumptions of Theorem 1 hold uniformly for $h_k \to 0$. Let $1 \leq p < \infty$ and $j = \min\{n, r\}$. Then, for every $u \in W^{j,p}(\Omega)$ there exists a sequence $u_k \in X_k$ such that $u_k \to u$.*

Proof. By the density of $C_c^\infty(\mathbb{R}^d)$ in $W^{j,p}(\Omega)$, there is a sequence of functions $v_i \in C_c^\infty(\mathbb{R}^d)$ whose restrictions to Ω converge to u in $W^{j,p}(\Omega)$. The corollary then follows by approximating each v_i by a sequence $u_{i_k} \in X_k$ and passing to a diagonal sequence. $\square$

4 Application to the Local Maximum-Entropy (LME) Approximation Scheme: Interior Estimates

In this Section, we specialize the results of Section 3 to the LME approximation schemes. We begin with a brief review of the definition and some of the properties of the Local Max-Ent Approximation scheme of Arroyo and Ortiz [2] (see also [3, 27] for a description of the method, and [24, 25, 26] for related work). We recall that a *convex approximation scheme* is a first-order consistent approximation scheme $\{I, W, P\}$ whose shape functions are non-negative. Convex approximation schemes satisfy a weak Kronecker-delta property at the boundary (cf. [2]), i. e., the approximation on the boundary of the domain does not depend on the nodal data over the interior points. This property simplifies the enforcement of essential boundary conditions. As pointed out in [2], in a convex approximation scheme the shape functions $w_a(x)$, $a \in I$, are well-defined if and only if $x \in \overline{\text{conv}}(P)$. Therefore, for such schemes to be feasible the domain Ω must be a subset of $\overline{\text{conv}}(P)$.

The Local Maximum-Entropy (LME) approximation scheme [2] is a convex approximation scheme that aims to satisfy two objectives simultaneously:

1. *Unbiased statistical inference* based on the nodal data.

2. Shape functions of *least width*.

Since for each point x, the shape functions of a convex approximation scheme are nonnegative and add up to 1, they can be thought of as the probability distribution of a random variable. The statistical inference of the shape functions is then measured by the *entropy* of the associated

probability distribution, as defined in information theory [22, 14, 15]. The entropy of a probability distribution p over I is:

$$H(p) = -\sum_{a \in I} p_a \log p_a, \tag{36}$$

where $0 \log 0 = 0$. The least biased probability distribution p is that which maximizes the entropy. In addition, the *width* of a non-negative function w about a point ξ is identified with the second moment

$$U_\xi(w) = \int_\Omega w(x)|x - \xi|^2 \, dx. \tag{37}$$

Thus, the width $U_\xi(w)$ measures how concentrated w is about ξ. According to this measure of width, the most local approximation scheme is that which minimizes the total width

$$U(W) = \sum_{a \in I} U_a(w_a) = \int_\Omega \sum_{a \in I} w_a(x)|x - x_a|^2 \, dx. \tag{38}$$

The Local Maximum-Entropy approximation schemes combine the functionals (36) and (38) into a single objective. More precisely, for a parameter $\beta > 0$, the LME approximation scheme is the minimizer of the functional

$$F_\beta(W) = \beta U(W) - H(W) \tag{39}$$

under the restriction of first-order consistency. Because of the local nature of this functional, it can be minimized pointwise, leading to the local convex minimization problem:

$$\left.\begin{array}{l} \min f_\beta(x, w(x)) = \displaystyle\sum_{a \in I} w_a(x)|x - x_a|^2 + \frac{1}{\beta} \sum_{a \in I} w_a(x) \log w_a(x), \\ \text{subject to: } w_a(x) \geq 0,\ a \in I, \quad \displaystyle\sum_{a \in I} w_a(x) = 1, \quad \sum_{a \in I} w_a(x) x_a = x. \end{array}\right\} \tag{LME}$$

In the limit of $\beta \to \infty$ the function f_β reduces to the power function of Rajan [19], whose minimizers define the piecewise-affine shape functions supported by the Delaunay triangulations associated with P.

Next we collect alternative characterizations of the LME shape functions based on duality theory. Let $Z \colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ be the *partition function*

$$Z(x, \lambda) = \sum_{a \in I} e^{-\beta|x - x_a|^2 + \langle \lambda(x), x - x_a \rangle} \tag{40}$$

of the point set. For every point $x \in \overline{\mathrm{conv}}(P)$, the problem (LME) has a unique solution $\{w_a^*(x) \colon a \in I\}$. Moreover, for every point $x \in \mathrm{conv}(P)$, the optimal shape functions $w_a^*(x)$ at x are of the form

$$w_a^*(x) = \frac{e^{-\beta|x - x_a|^2 + \langle \lambda^*(x), x - x_a \rangle}}{\sum_{b \in I} e^{-\beta|x - x_b|^2 + \langle \lambda^*(x), x - x_b \rangle}}, \tag{41}$$

where the vector $\lambda^*(x) \in \mathbb{R}^d$ minimizes the function

$$\log Z(x, \lambda) = \log \left(\sum_{a \in I} e^{-\beta|x - x_a|^2 + \langle \lambda, x - x_a \rangle} \right). \tag{42}$$

At points x belonging to the boundary of $\operatorname{conv} P$, the shape functions take expressions similar to (41) that solely involve the node points on the minimal face of $\overline{\operatorname{conv}}(P)$ that contains x. The gradient of $\log Z(x,\lambda)$ with respect to λ is

$$r(x,\lambda) \equiv \frac{\partial}{\partial\lambda} \log Z(x,\lambda) = \sum_{a\in I} w_a(x,\lambda)(x - x_a). \tag{43}$$

In addition, the Hessian of $\log Z(x,\lambda)$ with respect to λ follows as

$$J(x,\lambda) \equiv \frac{\partial^2}{\partial\lambda^2} \log Z(x,\lambda) = \sum_{a\in I} w_a(x,\lambda)(x - x_a) \otimes (x - x_a) - r(x,\lambda) \otimes r(x,\lambda). \tag{44}$$

Since $r(x,\lambda^*(x)) = 0$,

$$J^*(x) \equiv J(x,\lambda^*(x)) = \sum_{a\in I} w^*_a(x)(x - x_a) \otimes (x - x_a). \tag{45}$$

It can be shown that $J^*(x)$ is positive definite. In addition, the optimal shape functions $w^*_a \colon \operatorname{conv}(P) \to \mathbb{R}$ are C^∞ and have gradient

$$\nabla w^*_a(x) = -w^*_a(x)(J^*(x))^{-1}(x - x_a). \tag{46}$$

We refer the reader to [2] for the proofs of the preceding results and identities.

The following lemma shows that, for a point set P that is an h-covering of its closed convex hull $\overline{\operatorname{conv}}(P)$, and for every point $x \in \operatorname{conv}(P)$, for any vector $\lambda \neq 0$ there exists at least one node point x_λ in P that is close to x, and such that $x - x_\lambda$ is closely aligned with λ.

Lemma 2. *Let P be a finite point set that is an h-covering of its convex hull $\overline{\operatorname{conv}}(P)$ for some $h > 0$. Let x be a point in $\operatorname{conv}(P)$. Let $\varepsilon > 0$ be such that $\bar{B}(x,\varepsilon h) \subset \overline{\operatorname{conv}}(P)$. Let $\lambda \neq 0 \in \mathbb{R}^d$. Then, there exists a node point $x_\lambda \in P$ such that*

- *i)* $\varepsilon h \leq |x - x_\lambda| \leq (\varepsilon + 1)h$,
- *ii)* $|\lambda|\varepsilon h \leq \langle \lambda, x - x_\lambda \rangle$.

Proof. Let $\tilde{x}$ be the point $\tilde{x} = x - \frac{\varepsilon h}{|\lambda|}\lambda$. Since the distance between x and $\tilde{x}$ is εh, $\tilde{x} \in \bar{B}(x,\varepsilon h) \subset \overline{\operatorname{conv}}(P)$. In particular, since the point set P is an h-covering of $\overline{\operatorname{conv}}(P)$, there exists a d-simplex $T_{\tilde{x}}$ of size at most h, with vertices in P that contains $\tilde{x}$. Let $H^+ \subset \mathbb{R}^d$ be the halfspace $\{z \in \mathbb{R}^d \colon \langle \lambda, \tilde{x} - z \rangle \geq 0\}$. The point $\tilde{x}$ belongs to H^+. Moreover, since the d-simplex $T_{\tilde{x}}$ contains $\tilde{x}$, it follows that at least one extreme point of $T_{\tilde{x}}$ also belongs to H^+. Let x_λ be that extreme point. Note that x_λ is also a node point of P. We have the estimate

$$|x - x_\lambda| \leq |x - \tilde{x}| + |\tilde{x} - x_\lambda| \leq \varepsilon h + h = (\varepsilon + 1)h. \tag{47}$$

In addition, we have

$$|x - x_\lambda|^2 = |x - \tilde{x}|^2 + |\tilde{x} - x_\lambda|^2 + 2\langle x - \tilde{x}, \tilde{x} - x_\lambda \rangle. \tag{48}$$

By the definition of $\tilde{x}$, and since x_λ belongs to H^+, it follows that

$$\langle x - \tilde{x}, \tilde{x} - x_\lambda \rangle = \frac{\varepsilon h}{|\lambda|} \langle \lambda, \tilde{x} - x_\lambda \rangle \geq 0. \tag{49}$$

From this inequality and eq. (48) we obtain

$$|x - x_\lambda|^2 \geq |x - \tilde{x}|^2 = (\varepsilon h)^2, \tag{50}$$

or $|x - x_\lambda| \geq \varepsilon h$. Finally, from the definition of $\tilde{x}$ we have

$$\langle \lambda, x - \tilde{x} \rangle = |\lambda| \varepsilon h \tag{51}$$

and

$$\langle \lambda, x - x_\lambda \rangle = \langle \lambda, x - \tilde{x} \rangle + \langle \lambda, \tilde{x} - x_\lambda \rangle \geq |\lambda| \varepsilon h, \tag{52}$$

where we have used that x_λ belongs to H^+ and, hence, $\langle \lambda, \tilde{x} - x_\lambda \rangle \geq 0$. □

In view of (41), in order to verify that the LME shape functions have polynomial decay we require a bound on the minimizer $\lambda^*(x) \in \mathbb{R}^d$ of the partition function $Z(x, \lambda)$, eqs. (40) and (42). To this end, we begin with the following lemma.

Lemma 3. *Let P be a point set that is an h-covering of Ω with h-density bounded by τ, for some h, $\tau > 0$. Let $\beta = \frac{\gamma}{h^2}$ for some $\gamma > 0$. Then, there exists a constant c_Z that depends on γ, τ, and d, such that*

$$Z(x, 0) \leq c_Z \tag{53}$$

for every $x \in \mathrm{conv}(P)$.

Proof. For every nonnegative integer $t \geq 1$, let $U_t(x)$ be the subset of node points $U_t(x) = \{x_a \in P \colon (t-1)h \leq |x_a - x| < th\}$. Then, by Proposition 2 we have

$$\begin{aligned} Z(x,0) &= \sum_{a \in I} e^{-\beta |x - x_a|^2} = \sum_{t=1}^{\infty} \left(\sum_{x_a \in U_t(x)} e^{-\beta |x - x_a|^2} \right) \\ &\leq \sum_{t=1}^{\infty} \left(\# U_t(x) \, e^{-\beta (t-1)^2 h^2} \right) \leq \sum_{t=1}^{\infty} c t^{d-1} e^{-\gamma (t-1)^2} = c_Z. \end{aligned} \tag{54}$$

It is readily verified that the series of the right hand side is absolutely convergent. Moreover, because this series is defined in terms of γ, τ, and d, its limit c_Z also depends on γ, τ, and d only. □

By optimality, $\lambda^*(x)$ has the property that $Z(x, \lambda^*(x)) \leq Z(x, 0)$. This observation, combined with the upper bound on $Z(x, 0)$ of Lemma 3, suffices to estimate $|\lambda^*(x)|$.

Lemma 4. *Let P be a point set that is an h-covering of Ω with h-density bounded by τ, for some h, $\tau > 0$. Let $\beta = \frac{\gamma}{h^2}$ for some $\gamma > 0$ and $\varepsilon > 0$. Then, there exists a constant $c_\lambda > 0$ that depends on γ, τ, and d only such that*

$$|\lambda^*(x)| \leq \frac{c_\lambda}{\min\{\varepsilon, 1\} h} \tag{55}$$

for every point x such that $\bar{B}(x, \varepsilon h) \subset \overline{\mathrm{conv}}(P)$.

Proof. We note that, since log is an increasing function, $\lambda^*(x)$ also minimizes $Z(x,\lambda)$. Let $\varepsilon_2 = \min\{\varepsilon, 1\}$. We proceed to find a constant c_λ such that, if $|\lambda| \geq \frac{c_\lambda}{\varepsilon_2 h}$, then $Z(x,\lambda) > Z(x,0)$. To this end, let $\lambda \neq 0$ be a fixed vector. Since $\bar{B}(x, \varepsilon_2 h) \subset \overline{\text{conv}}(P)$ and since P is an h-covering of $\overline{\text{conv}}(P)$, by Lemma 2 there exists a point $x_\lambda \in P$ such that $\varepsilon_2 h \leq |x - x_\lambda| \leq (\varepsilon_2 + 1)h$ and $\langle \lambda, x - x_\lambda \rangle \geq |\lambda| \varepsilon_2 h$. Using these inequalities and noting that $\varepsilon_2 \leq 1$, we further obtain

$$Z(x,\lambda) = \sum_{a \in I} e^{-\beta|x-x_a|^2 + \langle \lambda, x - x_a \rangle} \geq e^{-\beta|x-x_\lambda|^2 + \langle \lambda, x - x_\lambda \rangle} \geq e^{-\beta(1+\varepsilon_2)^2 h^2 + \varepsilon_2 h |\lambda|} \geq e^{-4\gamma + \varepsilon_2 h |\lambda|}. \quad (56)$$

By Lemma 3, there exists a constant c_Z that depends on γ, τ, and d, such that $Z(x,0) \leq c_Z$. Combining this bound with eq. (56), it follows that a sufficient condition for λ not to be optimal is that $e^{-4\gamma + \varepsilon_2 h |\lambda|} > c_Z$ or, equivalently,

$$|\lambda| > \frac{\ln c_Z + 4\gamma}{\min\{\varepsilon, 1\} h} = \frac{c_\lambda}{\min\{\varepsilon, 1\} h}. \quad (57)$$

Therefore, (55) is a necessary condition for $\lambda^*(x)$ to be optimal. □

We note that, for fixed $\varepsilon > 0$ and for points x at distance ε or greater to the boundary of $\overline{\text{conv}}(P)$, the upper bound (55) is $\mathrm{O}(h^{-1})$. By contrast, for points $x \in \overline{\text{conv}}(P)$ arbitrarily close of the boundary of $\overline{\text{conv}}(P)$, the right hand side of (55) diverges. The following example shows that $|\lambda^*(x)|$ may indeed diverge near the boundary.

Example 1. Let $\Omega = [a,b] \subset \mathbb{R}$, $h = b - a$ and let $P = \{a, b\}$ be a point set of Ω. Let $\beta = \frac{\gamma}{h^2}$ for a some $\gamma > 0$. The optimality condition for $\lambda^*(x)$ is

$$\frac{\partial Z(x,\lambda)}{\partial \lambda} = e^{-\frac{\gamma}{h^2}(x-a)^2 + \lambda^*(x)(x-a)}(x-a) + e^{-\frac{\gamma}{h^2}(x-a-h)^2 + \lambda^*(x)(x-a-h)}(x-a-h) = 0. \quad (58)$$

For this condition we find

$$\lambda^*(x) = \frac{\log(a+h-x) - \log(x-a)}{h} + \frac{\gamma}{h^2}(2x - 2a - h). \quad (59)$$

For a fixed $0 < \varepsilon < 1$, and for points $x \in (a + \varepsilon h, a + h - \varepsilon h)$, we indeed have $|\lambda^*(x)| = \mathrm{O}(h^{-1})$. However, $\lim_{x \to a^+} \lambda^*(x) = \infty$, and $\lim_{x \to b^-} \lambda^*(x) = -\infty$. We note that the LME shape functions for this case reduce to

$$w_a^*(x) = \frac{a+h-x}{h}, \quad (60a)$$

$$w_b^*(x) = \frac{x-a}{h}. \quad (60b)$$

In particular, the shape functions and their derivatives are bounded in Ω even though the value of $|\lambda^*(x)|$ is unbounded at the boundary. From a computational perspective, this example suggests that computing the shape functions and their derivatives using Equations (42) and (41) may be unstable near the boundary, even if the shape functions and their derivatives are themselves well-behaved. In Section 5 we will examine the behavior of the shape functions near the boundary more thoroughly. □

The following lemma supplies the requisite estimate of the partition function Z.

Lemma 5. *Under the assumptions of Lemma 4, there exist constants m_Z, $M_Z > 0$ that depend on γ, τ, ε, and d only and such that*

$$m_Z \le Z(x, \lambda^*(x)) \le M_Z \tag{61}$$

for every point x such that $\bar{B}(x, \varepsilon h) \subset \overline{\text{conv}}(P)$.

Proof. By optimality, $Z(x, \lambda^*(x)) \le Z(x, 0)$ and, by Lemma 3, $Z(x, \lambda^*(x)) \le c_Z = M_Z$ for every $x \in \text{conv}(P)$. Since P is an h-covering of $\overline{\text{conv}}(P)$, there exists a point $x_0 \in P$ at distance to x less or equal to h. In addition, by Lemma 4, there exists a constant c_λ such that $|\lambda^*(x)| \le \frac{c_\lambda}{\varepsilon_2 h}$, where $\varepsilon_2 = \min\{\varepsilon, 1\}$. We thus have

$$Z(x, \lambda^*(x)) \ge e^{-\beta|x-x_0|^2 + \langle \lambda^*(x), x-x_0 \rangle} \ge e^{-\gamma - |\lambda^*(x)|\,|x-x_0|} \ge e^{-\gamma - \frac{c_\lambda}{\varepsilon_2}} = m_Z > 0, \tag{62}$$

as advertised. $\square$

Recall that $J^*(x) \in \mathbb{R}^{d\times d}$ is the Hessian of $\log Z(x, \lambda^*(x))$ with respect to λ, eq. (45). We proceed to estimate $\|J^*(x)^{-1}\|$.

Lemma 6. *Let P be a point set that is an h-covering of Ω with h-density bounded by τ, for some h, $\tau > 0$. Let $\beta = \frac{\gamma}{h^2}$ for some $\gamma > 0$. Let $\varepsilon > 0$. Let x be such that $\bar{B}(x, \varepsilon h) \subset \overline{\text{conv}}(P)$. Then, there exists a constant $c_{J^{-1}} > 0$ that depends on τ, γ, ε, and d such that*

$$\|J^*(x)^{-1}\| \equiv \sup_{y\neq 0} \frac{|J^*(x)^{-1}(y)|}{|y|} \le c_{J^{-1}} h^{-2}. \tag{63}$$

Proof. Let $u \neq 0$ be a fixed vector. Then, from eq. (45) we have

$$u^T J^*(x) u = \frac{\sum_{a\in I} e^{-\beta|x-x_a|^2 + \langle \lambda^*(x), x-x_a\rangle} \langle u, x-x_a\rangle^2}{Z(x, \lambda^*(x))}. \tag{64}$$

Next, we analyze the numerator and denominator of the right-hand side in turn. Let $\varepsilon_2 = \min\{\varepsilon, 1\}$. By Lemma 2, there exists a point $x_u \in P$ such that $\varepsilon_2 h \le |x - x_u| \le (\varepsilon_2 + 1)h$ and $\langle u, x - x_u\rangle \ge |u|\varepsilon_2 h$. Since $\bar{B}(x, \varepsilon h) \subset \overline{\text{conv}}(P)$, by Lemma 4 there exists a constant c_λ such that $|\lambda^*(x)| \le \frac{c_\lambda}{\varepsilon_2 h}$, and we have

$$|\langle \lambda^*(x), x - x_u\rangle| \le |\lambda^*(x)|\,|x - x_u| \le \frac{c_\lambda}{\varepsilon_2 h}(\varepsilon_2 + 1)h = \frac{c_\lambda}{\varepsilon_2}(\varepsilon_2 + 1). \tag{65}$$

Hence,

$$\begin{aligned} &\sum_{a\in I} e^{-\beta|x-x_a|^2 + \langle \lambda^*(x), x-x_a\rangle} \langle u, x - x_a\rangle^2 \\ &\ge e^{-\beta|x-x_u|^2 + \langle \lambda^*(x), x-x_u\rangle} \langle u, x - x_u\rangle^2 \ge e^{-(\varepsilon_2+1)^2\gamma - \frac{c_\lambda}{\varepsilon_2}(\varepsilon_2+1)} |u|^2 \varepsilon_2^2 h^2. \end{aligned} \tag{66}$$

where we write $\beta = \frac{\gamma}{h^2}$. Combining the bound supplied by Lemma 5 with eq. (66), we get

$$|u^T J^*(x) u| \ge e^{-(\varepsilon_2+1)^2\gamma - \frac{c_\lambda}{\varepsilon_2}(\varepsilon_2+1)} \frac{\varepsilon_2^2}{M_Z} |u|^2 h^2 = c_J |u|^2 h^2, \tag{67}$$

where $c_J = e^{-(\varepsilon_2+1)^2\gamma - \frac{c_\lambda}{\varepsilon_2}(\varepsilon_2+1)} \frac{\varepsilon_2^2}{M_Z} > 0$ depends on γ, τ, ε, and d only. Let $\lambda_{\min}(x)$ be the smallest eigenvalue of $J^*(x)$. Since $J^*(x)$ is positive-definite [2], it follows that $\lambda_{\min}(x) > 0$. Inequality (67) then implies that $\lambda_{\min}(x) \ge c_J h^2$. Since $\|J^*(x)^{-1}\| = 1/\lambda_{\min}(x)$, the estimate (63) follows immediately with $c_{J^{-1}} = 1/c_J$. $\square$

We are finally in a position to estimate the derivatives of the LME shape functions.

Proposition 5. *Let P be a point set that is an h-covering of Ω with h-density bounded by τ, for some h, $\tau > 0$. Let $\beta = \frac{\gamma}{h^2}$, for some $\gamma > 0$ and $\varepsilon > 0$. Let $W = \{w_a^*\colon a \in I\}$ be the optimal shape functions of the LME approximation scheme with node set P and parameter β. Then,*

$$|\nabla w_a^*(x)| \leq c_{J^{-1}}\, w_a^*(x)|x - x_a|\, h^{-2}, \tag{68}$$

for every point x such that $\bar{B}(x, \varepsilon h) \subset \overline{\mathrm{conv}}(P)$ and every point $x_a \in P$.

Proof. The estimate (68) follows immediately from Lemma 6 and eq. (46). □

Next we show that the LME approximation scheme has polynomial decay of order $(1, s)$ for every $s \geq 1$.

Proposition 6. *Let $\{I, W, P\}$ be an LME approximation scheme. Suppose that P is an h-covering of Ω, P has h-density bounded by τ, $\beta = \gamma/h^2$ for some $\gamma > 0$. Let $\varepsilon > 0$, and $s \geq 1$. Then, there exists a constant $c > 0$ (depending on d, γ, τ, ε, and s) such that the approximation scheme has polynomial decay of order $(1, s)$ for c and h in $\Omega_{\varepsilon h} = \{x \in \mathbb{R}^d$ s. t. $\bar{B}(x, \varepsilon h) \subset \overline{\mathrm{conv}}(P)\}$.*

Proof. We recall that the LME shape functions are C^∞ on $\mathrm{conv}(P)$ ([2]). Next, we show that there exists a constant $c > 0$ that depends on γ, τ, d, ε, and s, such that, for any k,

$$\sup_{|\alpha|\leq 1} \sup_{x\in\Omega_{\varepsilon h}} \sup_{a\in I} \left(1 + \left|\frac{x - x_a}{h}\right|^2\right)^s h^{|\alpha|}\, |D^\alpha w_a^*(x)| \leq c. \tag{69}$$

From Lemmas 4 and 5 we have

$$\begin{aligned} 0 \leq w_a^*(x) &= \frac{e^{-\beta|x-x_a|^2+\langle\lambda^*(x),x-x_a\rangle}}{Z(x,\lambda^*(x))} \\ &\leq \frac{e^{-\gamma|(x-x_a)/h|^2+|\lambda^*(x)||x-x_a|}}{m_Z} \leq \frac{e^{-\gamma|(x-x_a)/h|^2+\tilde{c}_\lambda|(x-x_a)/h|}}{m_Z}, \end{aligned} \tag{70}$$

with $\tilde{c}_\lambda = c_\lambda/\min\{\varepsilon, 1\}$. In addition,

$$\begin{aligned} &\sup_{x\in\Omega_{\varepsilon h}} \sup_{a\in I} \left(1 + \left|\frac{x - x_a}{h}\right|^2\right)^s w_a^*(x) \\ &\leq \sup_{x\in\Omega_{\varepsilon h}} \sup_{a\in I} \left(1 + \left|\frac{x - x_a}{h}\right|^2\right)^s \frac{e^{-\gamma|(x-x_a)/h|^2+\tilde{c}_\lambda|(x-x_a)/h|}}{m_Z} \\ &\leq c' := \sup_{t\geq 0} \left(1 + t^2\right)^s \frac{e^{-\gamma t^2+\tilde{c}_\lambda t}}{m_Z} < \infty, \end{aligned} \tag{71}$$

since $\frac{e^{-\gamma t^2+\tilde{c}_\lambda t}}{m_Z}$ is a rapidly decreasing function of t. We note that c' is defined in terms of the

constants d, γ, τ, ε, and s. Thus, by Proposition 5 we have

$$\begin{aligned}
&\sup_{x\in\Omega_{\varepsilon h}}\sup_{a\in I}\left(1+\left|\frac{x-x_a}{h}\right|^2\right)^s h\,|\nabla w_a^*(x)| \\
&\leq \sup_{x\in\Omega_{\varepsilon h}}\sup_{a\in I}\left(1+\left|\frac{x-x_a}{h}\right|^2\right)^s hc_{J-1}w_a^*(x)|x-x_a|h^{-2} \\
&\leq \sup_{x\in\Omega_{\varepsilon h}}\sup_{a\in I}\left(1+\left|\frac{x-x_a}{h}\right|^2\right)^s c_{J-1}w_a^*(x) < c_{J-1}c', \qquad (72)
\end{aligned}$$

as advertised. □

The next Theorem bounds uniformly the error of the approximate function u_k and its derivatives to a smooth function u and its derivatives. The result is based on Theorem 1 that holds for a general approximation scheme.

Theorem 2. *Under the assumptions of Proposition 6, let $u \in C^2(\bar{\Omega})$. Then, there exists a constant $C > 0$, that depends on γ, τ, ε, and d only, such that*

$$|D^\alpha u_I(x) - D^\alpha u(x)| \leq C\|D^2u\|_\infty h^{2-|\alpha|}, \qquad (73)$$

for $x \in \Omega_{\varepsilon h}$, $|\alpha| \leq 1$.

Proof. The theorem follows from Proposition 6 and Theorem 1. □

Finally, we are in a position to show that LME approximation spaces on a domain Ω' are dense in $W^{1,p}(\Omega)$ for subdomains $\Omega \subset \Omega'$ which are compactly contained in Ω'. This result is derived from the polynomial decay of LME schemes, and the density of approximation schemes of Corollary 2.

Corollary 3. *Let Ω be a domain satisfying the segment condition, and let Ω' be an auxiliary domain such that $\overline{\Omega} \subset \Omega'$. Let $\{I_k, W_k, P_k\}$ be a sequence of LME approximation schemes in Ω'. Suppose that the assumptions of Proposition 6 hold for $\{I_k, W_k, P_k\}$ in Ω' uniformly for $h_k \to 0$. Let $1 \leq p < \infty$. Then, for every $u \in W^{1,p}(\Omega)$ there exists a sequence $u_k \in X_k$ such that $u_{k|\Omega} \to u$.*

Proof. As $\overline{\Omega} \subset \Omega'$, there exists $r > 0$ such that, $\cup_{x\in\Omega}B(x,r) = \{x \in \mathbb{R}^d \colon \mathrm{dist}(x,\Omega) < r\} \subset \Omega'$. The sequence of approximation schemes $\{I_k, W_k, P_k\}$, when restricted to Ω, has uniform polynomial decay $(1,s)$ for any fixed s. Then, the theorem follows from Corollary 2. □

Corollary 3 guarantees the density of the LME approximates on $W^{1,p}(\Omega)$, provided that the sequence of LME approximation schemes $\{I_k, W_k, P_k\}$ is defined on a bigger domain Ω'. We note that, in this case, the LME scheme does not obey the weak Kronecker-delta property at the boundary of Ω, making it less straightforward to enforce boundary conditions on Ω. However, imposing boundary conditions can be done in this case by using standard Lagrangian multipliers, see e. g. [13, 8].

5 Application to the Local Maximum-Entropy (LME) Approximation Scheme: Estimates up to the Boundary

In Section 4 we have seen that, for a sequence $\{I_k, W_k, P_k\}$ of LME approximation schemes, we have density of the approximation space X_k in $W^{1,p}_{\mathrm{loc}}(\Omega)$. In order to treat boundary value problems, however, we need density results up to the boundary of Ω. A way to guarantee the density in $W^{1,p}(\Omega)$ is to work with a sequence $\{I_k, W_k, P_k\}$ defined on a (strictly) bigger domain Ω', as discussed in Corollary 3. In this section, we analyze the density of the approximation space X_k when the domain of the LME scheme is Ω.

While we will see that density can be extended to $W^{1,p}_0(\Omega)$ in general, a major technical difficulty with estimates up to the boundary comes from the fact that $\lambda^*(x)$ blows up as x approaches $\partial\Omega$. This blowup is indeed a manifestation of the weak Kronecker-delta property at the boundary, as λ^* will blow up in such a way that in the limit no weight is given to nodal data in the interior of Ω. For general Ω, this behavior can become very complicated and lead to blow up of the gradients of the optimal shape functions ∇w_a, with the result that the general convergence scheme of Section 3 is no longer applicable. Therefore, for simplicity we restrict attention to the class of polyhedral domains. Under generic assumptions, we shall obtain sufficiently strong estimates on ∇w^* near flat pieces of the boundary $\partial\Omega$ permitting to show that, away from a small singular part of the boundary, Sobolev functions can be approximated by linear combinations of shape functions in the limit of $h \to 0$. The singular boundary is of finite 2-capacity. With the help of a capacity argument we can then establish approximation results with truncated LME functions in $H^1(\Omega)$ for spatial dimension $d > 2$.

More precisely, in this section we will assume that Ω is a convex polytope in $\mathbb{R}^d$, P is an h-covering for Ω with $\operatorname{conv} P = \Omega$ such that there exists a constant $\eta > 0$ such that $\{x \in P \colon 0 < \operatorname{dist}(x, \partial\Omega) < \eta h\} = \emptyset$. Note that then $P \cap \partial\Omega$ is an h-covering for $\partial\Omega$.

Assume that $A = H \cap \partial\Omega$, H some hyperplane, is a flat $(d-1)$-dimensional subset of the boundary of Ω. With the aim to control $\nabla w^*(x)$ for x in the vicinity of A, our first task will be to exactly estimate the behavior of $J^*(x)$ in this regime. First note that with a proper choice of the coordinate system we may assume that $H = \{x_1 = 0\} = \{0\} \times \mathbb{R}^{d-1}$ with $\Omega \cap \{x_1 \geq 0\} = \Omega$. Accordingly, we write

$$\lambda^*(x) = (\lambda_1^*(x), \lambda'(x)) \in \mathbb{R} \times \mathbb{R}^{d-1} \tag{74}$$

and, for $x = (x_1, x')$,

$$Z = \sum_{a \in I} e^{-\beta|x - x_a|^2 + \langle \lambda', x' - x'_a \rangle + (x - x_a)_1 \lambda_1^*}. \tag{75}$$

We fix $\delta > 0$ and consider points $x \in \Omega$ with $x = (\rho, x') \in \mathbb{R} \times \mathbb{R}^{d-1}$ for ρ small such that $B_{\delta h}(0, x') \cap H = B_{\delta h}(0, x') \cap A$. In the following lemmas we will also set $h = 1$ for arbitrarily large Ω and recover the general case in Proposition 7 by rescaling afterwards. Generic positive constants, denoted c, c', c'' or C, C', will be independent of ρ and the size of Ω.

Lemma 7. *There is a constant $C > 0$ such that*

$$|\lambda'(x)| \leq C \quad \textit{and} \quad \lambda_1^*(x) \geq -C. \tag{76}$$

Proof. This result follows along the same lines as the proof of Lemma 4 for the boundedness of λ^* in the interior of Ω. $\square$

In order to investigate Z we split the sum as

$$Z = \sum_{a \in I_A} e^{-\beta|x-x_a|^2 + \langle \lambda', x'-x'_a \rangle + \rho\lambda_1^*} + \sum_{a \in I \setminus I_A} e^{-\beta|x-x_a|^2 + \langle \lambda', x'-x'_a \rangle - (x_a - x)_1 \lambda_1^*}, \tag{77}$$

where I_A collects those indices a for which $x_a \in A$.

Lemma 8. *As ρ tends to 0, $\lambda_1^* \to \infty$ such that $\rho\lambda_1^* \to 0$.*

Proof. Writing Z as in (77) and noting that $(x_a - x)_1 > \eta$ for $a \notin I_A$ and $\rho > 0$, we see that

$$Z \geq \sum_{a \in I_A} e^{-\beta|x-x_a|^2 + \langle \lambda', x'-x'_a \rangle} \tag{78}$$

and that this lower bound is in fact achieved only if $\rho\lambda_1^* \to 0$ and $\lambda_1^* \to \infty$. □

In particular, we see that Z still remains bounded from above and from below by positive constants.

In order to estimate J^*, we first observe that the optimality condition $\frac{\partial Z}{\partial \lambda_1} = 0$ implies

$$\rho \sum_{a \in I_A} e^{-\beta|x-x_a|^2 \langle \lambda', x'-x'_a \rangle + \rho\lambda_1^*} = \sum_{a \in I \setminus I_A} e^{-\beta|x-x_a|^2 + \langle \lambda', x'-x'_a \rangle - (x_a - x)_1 \lambda_1^*} (x_a - x)_1. \tag{79}$$

Lemma 9. *There is a constant $c > 0$ such that the first entry J_{11}^* in $J^*(x)$ satisfies*

$$J_{11}^* \geq c\rho. \tag{80}$$

Proof. Since $(x_a - x)_1 \geq \eta$ for $a \notin I_A$ we find by eq. (79) and Lemma 7

$$\begin{aligned} J_{11}^* &= \sum_{a \in I} w_a^*(x)(x - x_a)_1^2 \\ &\geq Z^{-1} \sum_{a \in I \setminus I_A} e^{-\beta|x-x_a|^2 + \langle \lambda', x'-x'_a \rangle - (x_a - x)_1 \lambda_1^*} (x_a - x)_1^2 \\ &\geq \eta Z^{-1} \sum_{a \in I \setminus I_A} e^{-\beta|x-x_a|^2 + \langle \lambda', x'-x'_a \rangle - (x_a - x)_1 \lambda_1^*} (x_a - x)_1 \\ &= \eta\rho Z^{-1} \sum_{a \in I_A} e^{-\beta|x-x_a|^2 + \langle \lambda', x'-x'_a \rangle + \rho\lambda_1^*} \\ &\geq c\rho \end{aligned} \tag{81}$$

for some constant $c > 0$. □

We now derive an upper bound for the entries of the first row and column of J^*.

Lemma 10. *For any $0 < \mu < 1$ there exists a constant $C > 0$ such that*

$$|J_{1j}^*| = |J_{j1}^*| \leq C\rho^\mu, \qquad j = 1, \ldots, d. \tag{82}$$

Proof. For $j = 1, \dots, d$ we have $J^*_{1j} = J^*_{j1} = \sum_{a \in I} w^*_a(x)(x - x_a)_1 (x - x_a)_j$. First summing over $a \in I_A$ gives the obvious bound

$$\begin{aligned} \left| \sum_{a \in I_A} w^*_a(x)(x - x_a)_1 (x - x_a)_j \right| &\le Z^{-1} \sum_{a \in I_A} e^{-\beta |x - x_a|^2 + \langle \lambda', x' - x'_a \rangle + \rho \lambda^*_1} \rho |x - x_a| \\ &\le C\rho. \end{aligned} \tag{83}$$

In order to estimate the remaining sum, we let $p = \frac{1}{\mu}$ and choose $1 < q < \infty$ with $\frac{1}{p} + \frac{1}{q} = 1$, so that

$$\left| \sum_{a \in I \setminus I_A} w^*_a(x)(x - x_a)_1 (x - x_a)_j \right| \le \left(\sum_{a \in I \setminus I_A} w^*_a(x)(x_a - x)_1^p \right)^{\frac{1}{p}} \left(\sum_{a \in I \setminus I_A} w^*_a(x) |x - x_a|_j^q \right)^{\frac{1}{q}} \tag{84}$$

by Hölder's inequality. Here the second factor in (84) is bounded by

$$\left(Z^{-1} \sum_{a \in I \setminus I_A} e^{-\beta |x - x_a|^2 + \langle \lambda', x' - x'_a \rangle - (x_a - x)_1 \lambda^*_1} |x - x_a|_j^q \right)^{\frac{1}{q}} \le C, \tag{85}$$

see Lemma 7. To estimate the first factor we note that, since P is a 1-covering of Ω, there exists $\bar{a} \in I \setminus I_A$ such that

$$|x_{\bar{a}} - x| \le C'$$

for a constant $C' > \eta$. For ρ sufficiently small and thus λ^*_1 sufficiently large, we then have the estimate

$$\begin{aligned} \sum_{\substack{a \in I \setminus I_A \\ (x_a - x)_1 \ge C'}} w^*_a(x)(x_a - x)_1^p &\le Z^{-1} \sum_{\substack{a \in I \setminus I_A \\ (x_a - x)_1 \ge C'}} e^{-\beta |x - x_a|^2 + \langle \lambda', x' - x'_a \rangle - C' \lambda^*_1} (x_a - x)_1^p \\ &\le C Z^{-1} e^{-C' \lambda^*_1} \\ &\le C Z^{-1} e^{-\beta |x - x_{\bar{a}}|^2 + \langle \lambda', x' - x'_{\bar{a}} \rangle - (x_{\bar{a}} - x)_1 \lambda^*_1} \\ &\le C Z^{-1} \eta^{-1} \sum_{a \in I \setminus I_A} e^{-\beta |x - x_a|^2 + \langle \lambda^*, x - x_a \rangle} (x_a - x)_1, \end{aligned} \tag{86}$$

as $(x_a - x)_1 \ge \eta$ for $a \in I \setminus I_A$. On the other hand, for a with $(x_a - x)_1 \le C'$ we have the bound

$$(x_a - x)_1^p \le C (x_a - x)_1. \tag{87}$$

Combining the two last estimates, we see that the term in the first factor of (84) satisfies

$$\sum_{a \in I \setminus I_A} w^*_a(x)(x - x_a)_1^p \le C \sum_{a \in I \setminus I_A} w^*_a(x)(x - x_a)_1. \tag{88}$$

Since by (79) this last expression is bounded by $C\rho$, we arrive at

$$\left| \sum_{a \in I \setminus I_A} w^*_a(x)(x - x_a)_1 (x - x_a)_j \right| \le C \rho^{\frac{1}{p}} = C \rho^{\mu} \tag{89}$$

by (84). Together with the bound (83) for the first part of the sum we have shown that indeed

$$|J_{1i}^*| \le C\rho^{\mu}.$$

□

For the remaining part $B = (J_{ij}^*)_{2\le i,j\le n}$ of the matrix J^* we obtain the following lower matrix bound.

Lemma 11. *There is a constant $c > 0$ such that*

$$B \ge c\,\mathrm{Id}_{n-1}\,. \tag{90}$$

Proof. As $P \cap H$ is a 1-covering for A, there is a set $J = \{a_1, \dots, a_{d-1}\} \subset I_A$ of $d-1$ points such that $c' \le |x' - x'_a| \le c''$ and $\det(x' - x'_{a_1}, \dots, x' - x'_{a_{d-1}}) \ge c'$ for suitable constants c' and c''. Then

$$\begin{aligned} B &= \sum_{a\in I} w_a^*(x)(x' - x'_a) \otimes (x' - x'_a) \\ &\ge Z^{-1} \sum_{a\in J} e^{-\beta|x - x_{\bar a}|^2 + \langle \lambda', x' - x'_{\bar a}\rangle + \rho\lambda_1^*}(x' - x'_a) \otimes (x' - x'_a) \\ &\ge c \sum_{a\in J} (x' - x'_a) \otimes (x' - x'_a) \\ &\ge c\,\mathrm{Id}_{d-1} \end{aligned} \tag{91}$$

since all the projections $(x' - x'_a) \otimes (x' - x'_a)$ are nonnegative. □

As a consequence of the above results, we obtain an estimate for the inverse matrix $(J^*)^{-1} = (\tilde J_{ij})$.

Lemma 12. *For any $0 < \mu < \frac{1}{2}$ there exists a constant C such that*

$$|\tilde J_{ij}| \begin{cases} \le C\rho^{-1} & \text{for } i = j = 1, \\ \le C\rho^{-\mu} & \text{for } i = 1, j = 2, \dots, d \text{ or } j = 1, i = 2, \dots, d \quad \text{and} \\ \le C & \text{for } i, j = 2, \dots, d. \end{cases} \tag{92}$$

Proof. First note that, expanding with respect to the first row, for $\frac{1}{2} < \tilde\mu < 1$ we have

$$\det J^* = J_{11}^* \det B + O(\rho^{2\tilde\mu}) = J_{11}^* \det B \ge cJ_{11}^* \ge c\rho \tag{93}$$

by Lemmas 9, 10 and 11. Furthermore, as $|J^*| \le C$, we have

$$|(\operatorname{cof} J^*)_{ij}| \begin{cases} = |\det B| \le C & \text{for } i = j = 1, \\ \le C\rho^{\tilde\mu} & \text{for } i = 1, j \ge 2 \text{ or } j = 1, i \ge 2 \quad \text{and} \\ \le C(J_{11}^* + \rho^{2\tilde\mu}) & \text{for } i, j \ge 2. \end{cases} \tag{94}$$

for C sufficiently large. Now, Cramer's rule

$$(J^*)^{-1} = (\det J^*)^{-1} (\operatorname{cof} J^*)^T \tag{95}$$

implies

$$|\tilde{J}_{ij}| \begin{cases} \leq C\rho^{-1} & \text{for } i = j = 1, \\ \leq C\rho^{\tilde{\mu}-1} & \text{for } i = 1, j \geq 2 \text{ or } j = 1, i \geq 2 \quad \text{and} \\ \leq C & \text{for } i, j \geq 2 \end{cases} \tag{96}$$

and thus the assertion follows by choosing $\tilde{\mu}$ such that $\mu = 1 - \tilde{\mu}$. $\square$

Lemma 13. *For any $s > 0$ and $0 < \mu < \frac{1}{2}$ there is a constant $C > 0$ such that*

$$\left(1 + |x - x_a|^2\right)^s |\nabla w_a^*(x)| \leq C(1 + \rho^{-\mu}|x - x_a|). \tag{97}$$

Proof. If $a \in I_A$, then $x - x_a = (\rho, x' - x'_a)$ and Lemma 12 shows

$$\left|(J^*)^{-1}(x - x_a)\right| \leq C(1 + \rho^{-\mu}|x' - x'_a|) \leq C(1 + \rho^{-\mu}|x - x_a|). \tag{98}$$

So, by (46),

$$|\nabla w_a^*(x)| \leq C|w_a^*(x)|(1 + \rho^{-\mu}|x - x_a|). \tag{99}$$

Now, using that $(1 + |x - x_a|^2)^s|w_a^*(x)| \leq C$ for any a, we see that the estimate holds true for $a \in I_A$.

On the other hand, if $a \notin I_A$, then Lemma 12 only gives

$$\left|(J^*)^{-1}(x - x_a)\right| \leq C\rho^{-1}|x - x_a|, \tag{100}$$

whence

$$|\nabla w_a^*(x)| \leq C|w_a^*(x)|\rho^{-1}|x - x_a|. \tag{101}$$

But since $(x_b - x)_1 \geq \eta$ for all $b \notin I_A$, we also get

$$\begin{aligned} &(1 + |x - x_a|^2)^s|w_a^*(x)| \\ &= (1 + |x - x_a|^2)^s Z^{-1} e^{-\beta|x-x_a|^2 + \langle\lambda', x'-x'_a\rangle - (x_a - x)_1\lambda_1^*} \\ &\leq Z^{-1}\eta^{-1} \sum_{b \in I \setminus I_A} e^{-\beta|x-x_b|^2 + \langle\lambda', x'-x'_b\rangle - (x_b - x)_1\lambda_1^*}(x_b - x)_1(1 + |x - x_b|^2)^s. \end{aligned} \tag{102}$$

This term can now be estimated by $C\rho^{\tilde{\mu}}\rho^{-1}$ for $0 < \tilde{\mu} < 1$ precisely as the left hand side of (84) in Lemma 10, which leads to

$$(1 + |x - x_a|^2)^s|\nabla w_a^*(x)| \leq C\rho^{-\mu}|x - x_a| \tag{103}$$

for $0 < \mu < 1$. $\square$

Undoing the rescaling of h we can now summarize the previous lemmas in the following proposition the boundary behavior of ∇w_a^* near flat parts of $\partial\Omega$.

Proposition 7. *Suppose $x = (\rho, x') \in \mathbb{R} \times \mathbb{R}^{d-1}$ is such that $B_{\delta h}(0, x') \cap H = B_{\delta h}(0, x') \cap A$ for a boundary $(d-1)$-face $A = \partial\Omega \cap H$. Let $s > 0$ and $0 < \mu < \frac{1}{2}$. There is a constant $C > 0$ such that*

$$\left(1 + \left|\frac{x - x_a}{h}\right|^2\right)^s h|\nabla w^*_{a,h}(x)| \le C\left(1 + h^\mu \mathrm{dist}^{-\mu}(x, \partial\Omega)\right). \tag{104}$$

Proof. If P is an h-covering for Ω, then $h^{-1}P$ is a 1-covering for $h^{-1}\Omega$. Using subscripts h to highlight the dependence on h, we have

$$\begin{aligned} Z_h(x) &= \sum_{x_b \in P} e^{-\frac{\gamma}{h^2}|x-x_b|^2 + \langle \lambda^*_{(h)}, x - x_b\rangle} \\ &= \sum_{x_b \in P} e^{-\gamma|\frac{x-x_b}{h}|^2 + \langle h\lambda^*_{(h)}, \frac{x-x_b}{h}\rangle} \\ &= \sum_{x_b \in h^{-1}P} e^{-\gamma|\frac{x}{h}-x_b|^2 + \langle h\lambda^*_{(h)}, \frac{x}{h}-x_b\rangle}. \end{aligned} \tag{105}$$

This expression is minimized at $h\lambda^*_{(h)}(x) = \lambda^*_{(1)}(\frac{x}{h})$. For the shape functions $w^*_{a,h}$ we denote by $w_{a,1}$ the shape function corresponding to the node $\frac{x_a}{h} \in h^{-1}P$ and obtain

$$\begin{aligned} w^*_{a,h}(x) &= \frac{e^{-\frac{\gamma}{h^2}|x-x_a|^2 + \langle \lambda^*_{(h)}, x-x_a\rangle}}{\sum_{x_b \in P} e^{-\frac{\gamma}{h^2}|x-x_b|^2 + \langle \lambda^*_{(h)}, x-x_b\rangle}} \\ &= \frac{e^{-\gamma|\frac{x-x_a}{h}|^2 + \langle h\lambda^*_{(h)}, \frac{x-x_a}{h}\rangle}}{\sum_{x_b \in P} e^{-\gamma|\frac{x-x_b}{h}|^2 + \langle h\lambda^*_{(h)}, \frac{x-x_b}{h}\rangle}} \\ &= \frac{e^{-\gamma|\frac{x}{h}-\frac{x_a}{h}|^2 + \langle \lambda^*_{(1)}(\frac{x}{h}), \frac{x}{h}-\frac{x_a}{h}\rangle}}{\sum_{x_b \in h^{-1}P} e^{-\gamma|\frac{x}{h}-x_b|^2 + \langle \lambda^*_{(1)}(\frac{x}{h}), \frac{x}{h}-x_b\rangle}} \\ &= w^*_{a,1}\left(\frac{x}{h}\right). \end{aligned} \tag{106}$$

Applying Lemma 13 to $w^*_{a,1}$ we therefore obtain

$$\begin{aligned} \left(1 + \left|\frac{x - x_a}{h}\right|^2\right)^s |\nabla w^*_{a,h}(x)| &= \left(1 + \left|\frac{x - x_a}{h}\right|^2\right)^s h^{-1}\left|\nabla w^*_{a,1}\left(\frac{x}{h}\right)\right| \\ &\le Ch^{-1}\left(1 + \mathrm{dist}^{-\mu}\left(\frac{x}{h}, A\right)\left|\frac{x}{h} - \frac{x_a}{h}\right|\right). \end{aligned} \tag{107}$$

From our previous calculations we know already that the left hand side is bounded by a constant away from the boundary of Ω. Suppose x is such that $\mathrm{dist}^{-\mu}(\frac{x}{h}, A) \ge 1$. Since s is arbitrary we can absorb the last factor on the right hand side into the prefactor of the left hand side and finally obtain

$$\left(1 + \left|\frac{x - x_a}{h}\right|^2\right)^s h|\nabla w^*_{a,h}(x)| \le C\left(1 + h^\mu \mathrm{dist}^{-\mu}(x, \partial\Omega)\right). \tag{108}$$

$\square$

Now suppose that x is a general point near a possibly lower dimensional edge of $\partial\Omega$. More precisely, x is close to an m-face of A of $\partial\Omega$, which is the intersection of $d-m$ hyperplanes $H_1, \ldots, H_{d-m}$ with linearly independent normals which constitute $\partial\Omega$ in the vicinity of x.

Lemma 14. *There exists $R > 0$ such that for all $x_a \in P$ with* $\operatorname{dist}(x_a, \partial\Omega) \geq Rh$

$$\left(1 + \left|\frac{x - x_a}{h}\right|^2\right)^s h|\nabla w^*_{a,h}(x)| \leq 1. \tag{109}$$

Proof. We first assume again that $h = 1$. Let H be the hyperplane containing x which is perpendicular to λ^*. Similarly as in Lemma 7 we see that, as $\operatorname{dist}(x, A) \to 0$, $|\lambda^*|$ tends to infinity such that the projection of λ^* onto $\bigcap H_i$ remains bounded and that there are constants c, $C > 0$ such that

$$\left\langle y - x, \frac{\lambda^*}{|\lambda^*|} \right\rangle = \operatorname{dist}(y - x, H) \geq c \operatorname{dist}(y, H_1 \cup \ldots \cup H_{d-m}) - C \tag{110}$$

for every $y \in \Omega$.

Choose a set $J = \{a_1, \ldots, a_d\} \subset I$ of d points such that $c' \leq |x - x_a| \leq c''$ and $\det(x - x_{a_1}, \ldots, x - x_{a_d}) \geq c'$ for suitable constants c' and c''. Then

$$J^* \geq Z^{-1} \sum_{a \in J} e^{-\beta|x - x_a|^2 + \langle \lambda^*, x - x_a \rangle} (x - x_a) \otimes (x - x_a) \geq c\, e^{-C|\lambda^*|} \operatorname{Id}_{d-1} \tag{111}$$

since all the projections $(x - x_a) \otimes (x - x_a)$ are nonnegative. It follows that

$$(J^*)^{-1} \leq C e^{C|\lambda^*|} \operatorname{Id}_{d-1}. \tag{112}$$

Now if $x_a \in \Omega$ satisfies $\operatorname{dist}(x, \partial\Omega) \geq R$, then

$$\langle x - x_a, \lambda^* \rangle \leq -(c \operatorname{dist}(x_a, H_1 \cup \ldots \cup H_{d-m}) + C)|\lambda^*| \leq (-cR + C)|\lambda^*|. \tag{113}$$

So

$$|w^*_a| \leq Z^{-1} e^{-\beta|x - x_a|^2 + \langle \lambda^*, x - x_a \rangle} \leq Z^{-1} e^{-\beta|x - x_a|^2 - (cR - C)|\lambda^*|}. \tag{114}$$

It follows from (46) that

$$\begin{aligned} \left(1 + |x - x_a|^2\right)^s |\nabla w^*_a(x)| &\leq C \left(1 + |x - x_a|^2\right)^s e^{-\beta|x - x_a|^2 - (cR + C)|\lambda^*|} e^{C|\lambda^*|} |x - x_a| \\ &\leq C e^{(2C - cR)|\lambda^*|} \leq 1 \end{aligned} \tag{115}$$

for R sufficiently large, which proves the Lemma for $h = 1$. The estimate for general h now follows directly by rescaling as before. □

We are now in a position to prove our main density results up to the boundary. Density in $W_0^{1,p}(\Omega)$ in fact only relies on our previous interior estimates, see Section 4, and Lemma 14 and is true for general, not necessarily polyhedral domains Ω.

Theorem 3. *Let Ω be a bounded polyhedron and $\{I_k, W_k, P_k\}$ be a sequence of LME approximation schemes satisfying the assumptions of Proposition 6 uniformly for $h_k \to 0$. Then for any $u \in W_0^{1,p}(\Omega)$, $1 \leq p < \infty$, there exists a sequence $u_k \in X_k$ such that $u_k \to u$.*

Proof. It suffices to consider $u \in C_c^\infty(\Omega)$. Let $u_k = u_{I_k}$. By Proposition 3 we have

$$|D^\alpha u_k(x) - D^\alpha u(x)| \leq \sum_{a\in I} |R_2(x_a, x)| D^\alpha w_a^*(x)|, \tag{116}$$

which for $\operatorname{dist}(x, \partial\Omega) \geq \varepsilon h$ can be estimated by $C\|D^2 u\|_\infty h_k^{2-|\alpha|} \to 0$ as $h_k \to 0$, see Theorem 1.

If $\operatorname{dist}(x, \partial\Omega) \leq \varepsilon h$, then with the help of Lemma 14 precisely the same arguments as in the proof of Theorem 1 show that

$$\sum_{\substack{a\in I\\ |x-x_a|\geq Rh}} |R_2(x_a, x)| D^\alpha w_a^*(x)| \leq C\|D^2 u\|_\infty h_k^{2-|\alpha|} \to 0 \tag{117}$$

for a sufficiently large constant $R > 0$. But the remaining part of the sum vanishes for small h_k as $R_2(x_a, x) = 0$ if $|x - x_a| < Rh$, since then u vanishes on a neighborhood of the segment $\{x_a + \theta(x - x_a) \colon \theta \in [0, 1]\} \subset \{x \in \Omega \colon \operatorname{dist}(x, \partial\Omega) \leq (R + \varepsilon)h_k\}$. ☐

In order to formulate our main result on density up to the boundary we denote by $\partial_*\Omega$ the union of the interiors of the $(d-1)$-faces of $\partial\Omega$. ($\partial_*\Omega$ is the reduced boundary in the language of geometric measure theory.) The part of Ω a distance εh away from the singular boundary $\partial\Omega \setminus \partial_*\Omega$ is denoted $\tilde{\Omega}_{\varepsilon h} = \{x \in \Omega \colon \operatorname{dist}(x, \partial\Omega \setminus \partial_*\Omega) \geq \varepsilon h\}$.

Theorem 4. *Let Ω be a bounded polyhedron and $\{I_k, W_k, P_k\}$ be a sequence of LME approximation schemes satisfying the assumptions of Proposition 6 uniformly for $h_k \to 0$. Let $\varepsilon > 0$. Then for any $u \in W^{1,p}(\Omega)$, $1 \leq p < \infty$, there exists a sequence $u_k \in X_k$ such that $\|u_k - u\|_{W^{1,p}(\tilde{\Omega}_{\varepsilon h})} \to 0$.*

Therefore, density holds away from the singular boundary.

Proof. Let $u \in C^2(\Omega)$. As in the proof of Theorem 3 we find by Proposition 3 and the arguments in the proof of Theorem 1 that for all $x \in \tilde{\Omega}_{\varepsilon h}$

$$|D^\alpha u_I(x) - D^\alpha u(x)| \leq C\|D^2 u\|_\infty h^{2-|\alpha|} \left(1 + h^\mu \operatorname{dist}^{-\mu}(x, \partial\Omega)\right), \tag{118}$$

$0 < \mu < \frac{1}{2}$, where in addition we have applied Proposition 7 in order to estimate ∇w_a^* near the regular boundary. Consequently,

$$\begin{aligned}
\int_{\tilde{\Omega}_{\varepsilon h}} |D^\alpha u_I(x) - D^\alpha u(x)|^p \, dx &\leq Ch^{(2-|\alpha|)p} \int_{\tilde{\Omega}_{\varepsilon h}} 1 + h^{p\mu} \operatorname{dist}^{-p\mu}(x, \partial\Omega) \, dx \\
&\leq Ch^{(2-|\alpha|)p} \left(1 + h^{p\mu} \int_0^1 t^{-p\mu} \, dt\right) \\
&= Ch^{(2-|\alpha|)p}
\end{aligned} \tag{119}$$

for μ sufficiently close to 0. ☐

Note that since the $(d-2)$-dimensional Hausdorff measure of $\partial\Omega \setminus \partial_*\Omega$ is finite, this set has zero 2-capacity for $d \geq 3$. Theorem 4 thus shows that u can be approximated by $u_k \in X_k$ in H^1 up to sets of arbitrarily small 2-capacity. With the help of a capacity argument we obtain from Theorem 4.

Corollary 4. *Let Ω be a bounded polyhedron and $\{I_k, W_k, P_k\}$ be a sequence of LME approximation schemes, $\varepsilon > 0$. Suppose $d > 2$. Then for any $u \in H^1(\Omega)$ there exists a sequence $\chi_k \in H^1$ with $\chi_k \to 1$ in H^1 and a sequence $u_k \in X_k$ such that $\chi_k u_k \to u$ in H^1.*

Proof. Since the $(d-2)$ dimensional Hausdorff measure of the singular part $\partial\Omega\setminus\partial_*\Omega$ of the boundary is finite, this set has zero 2-capacity:

$$\mathrm{Cap}_2(\partial\Omega \setminus \partial_*\Omega) = 0. \tag{120}$$

In particular, for every neighborhood V of $\partial\Omega \setminus \partial_*\Omega$ and $\delta > 0$ there exists a function $\psi_\delta \in H^1(\mathbb{R}^d)$ with compact support in V such that $\psi_\delta > 1$ in a smaller neighborhood of $\partial\Omega \setminus \partial_*\Omega$ and

$$\int_{\mathbb{R}^d} |\nabla\psi_\delta|^2 \, dx < \delta. \tag{121}$$

(This follows, e. g., from Theorem 3 and its proof in [11, pp. 155–157].) By replacing, if necessary, ψ_δ with a mollification of $\max\{\min\{\psi_\delta, 1\}, -1\}$ we may assume that ψ_δ is smooth, $|\psi_\delta| \le 1$ and in particular $\psi_\delta \equiv 1$ near $\partial\Omega \setminus \partial_*\Omega$.

Now suppose $u \in C^1(\bar\Omega)$. By Theorem 4 we find $u_k \in X_k$ with $\|u_k - u\|_{W^{1,p}(\tilde\Omega_{h_k})} \to 0$ for all $p < \infty$. Since $1 - \psi_\delta$ vanishes in a neighborhood of $\partial\Omega \setminus \partial_*\Omega$, it follows that

$$\begin{aligned} \|(1-\psi_\delta)(u_k - u)\|^2_{H^1(\Omega)} &\le \|1-\psi_\delta\|^2_{L^\infty(\Omega)} \|u_k - u\|^2_{H^1(\tilde\Omega_{h_k})} + \|\nabla\psi_\delta\|_{L^2(\Omega)} \|u_k - u\|^2_{L^\infty(\tilde\Omega_{h_k})} \\ &\to 0 \end{aligned} \tag{122}$$

by Sobolev embedding. As

$$\begin{aligned} \|(1-\psi_\delta)u - u\|^2_{H^1} &= \|\psi_\delta u\|^2_{H^1} \\ &\le \int_V |u|^2 \, dx + \int_V |\nabla u|^2 \, dx + \|u\|^2_\infty \int_V |\nabla\psi_\delta|^2 \, dx \\ &\le C(|V| + \delta) \end{aligned} \tag{123}$$

and V and δ can be chosen arbitrarily small, by choosing diagonal sequences we see that every $u \in C^1(\bar\Omega)$ and hence in fact every $u \in H^1(\Omega)$ can be approximated by sequences $(1 - \psi_{\delta_k})u_k$, $u_k \in X_k$. □

6 Concluding remarks

The preceding analysis shows that, whereas the density of the LME approximating scheme in the interior of the domain follows directly from the general results for meshfree approximation schemes, the density of the scheme up to the boundary is a matter of considerable delicacy. This situation strongly suggests relaxing the positivity constraint and allowing for signed basis functions. This relaxation is also required for the formulation of higher-order approximation schemes, as noted by [2, 9]. Indeed, in the finite-element limit shape functions of quadratic order and higher are signed functions in general. As an additional bonus, signed shape functions enable the consideration of general—not necessarily convex—domains. These extensions are pursued in a follow-up publication [4], where LME-type approximation schemes of arbitrary order and smoothness are derived and their convergence properties are analyzed using the general analysis framework developed in this paper.

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